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Unquenched simulations of four-nucleon interactions

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Abstract

Exploratory simulations of four-nucleon interactions are performed taking into account the dynamical effects of internal nucleon loops. The four-nucleon interactions in the isoscalar and isovector channels are described by Yukawa interactions with auxiliary scalar fields. The nucleon mass and the average field lengths of the scalar fields are determined as a function of nucleon hopping parameter and Yukawa coupling strengths. There are no problems with "exceptional configurations" at strong couplings which make quenched simulations unreliable.

1 Introduction

There are impressive recent developments in solving QCD for the lightest nuclei, using the numerical technique of Lattice QCD (LQCD) (for recent reviews see [1, 2]). In the QCD-approach the nucleons are described as bound states of quarks and gluons and the nuclei are composed out of these composite objects. For nuclei heavier than, say, the helium an approach based on quarks and gluons would require a tremendous computing power beyond the exaflops-scale. However, in order to compute, for instance, binding energies of heavier nuclei it is also not clear whether one has to stick to the fundamental theory, because the relevant degrees of freedom are not quarks and gluons but nucleons, pions and other hadrons described in a chiral effective theory [3, 4].

The chiral effective theory can be taken as a starting point for applying non-perturbative lattice thechniques for nuclear physics. A lattice approach to nuclear physics was presented

in a row of papers by the authors of [5]-[11]. For an overview over the various available approaches and methods to nuclear physics using chiral effective theories see the recent review articles [12]-[14]. The approach taken in these publications differs fundamentally from the methods applied in LQCD simulations where the path integral in Euclidean space-time is simulated using Monte Carlo methods.

Recently, the application of Monte Carlo methods of LQCD has also been tried in [15] (for an earlier attempt see also [16]). In Ref. [15] two-nucleon binding energies have been calculated in the so called *quenched approximation* to the pionless effective field theory with isoscalar and isovector auxiliary scalar fields. In this approximation the fermion determinant in the path integral is replaced by a constant, i.e. internal fermion loops are neclected and hence no dynamical effects of the fermions are taken into account. Apart from being only an approximation to the Euclidean path integral, the quenched approximation suffers from the so called *exceptional configurations* – well known also from lattice QCD [17, 18]. Such field configurations have extremely small eigenvalues of the fermion matrix and hence give huge contributions to some expectation values and completely spoil the statistics. As is has been concluded in Ref. [15], in the effective field theory for nuclear interactions the occurence of exceptional configurations make quenched simulations impossible for strong couplings (actually for bare couplings in the range $\max(|C_0|, |C_1|) \geq 0.3$). This phenomenon has also been observed earlier in quenched simulations of some simpler Yukawa-models in [19]-[22]. Since this problem does not appear in numerical simulations of Yukawa models with dynamical fermions [23, 24], it can be expected that it does also disappear in nuclear Yukawa models if dynamical nucleons are included in the simulation update.

In this paper the results of first unquenched Euclidean Monte Carlo simulations are presented in the model studied previously in [15] with particular emphasis on the strong coupling region $\max(|C_0|, |C_1|) \geq 0.3$. After defining the lattice action and shortly describing the numerical simulation algorithm in Section 2, the results are presented. Conclusions and the discussion of the outlook for future work are contained in Section 3.

2 Numerical simulations

2.1 Lattice action and updating

The four-nucleon interactions are described here, as in Ref. [15] by Yukawa-couplings of the nucleon field to auxiliary scalar fields with isospin 0 ($\phi_x^{(0)}$) and 1 ($\phi_{ax}^{(1)}$ $(a = 1, 2, 3)$). The nucleon fields are described by a pair of Grassmann variables and are denoted by $\psi_{\alpha x}$ and

$\tilde{\psi}_{\alpha x}$ where $\alpha = 1, 2$ is the isospin index. The lattice action is defined by

$$S = S_N + S_{NA}\,. \tag{1}$$

where S_N is the Wilson fermion lattice action [25] with the nucleon hopping parameter κ:

$$S_N = \sum_x \left\{ (\tilde{\psi}_x \psi_x) - \kappa \sum_{\mu=\pm 1}^{\mu=\pm 4} (\tilde{\psi}_{x+\hat{\mu}}[1+\gamma_\mu]\psi_x) \right\}\,. \tag{2}$$

and the scalar part of the action contains the Yukawa-type couplings to the nucleon field:

$$S_{NA} = \sum_x \left\{ \phi_x^{(0)}\phi_x^{(0)} + \phi_{ax}^{(1)}\phi_{ax}^{(1)} + C_0\,\phi_x^{(0)}\,(\tilde{\psi}_x\psi_x) + C_1\,\phi_{ax}^{(1)}\,(\tilde{\psi}_x\tau_a\psi_x) \right\}\,. \tag{3}$$

Here C_0 and C_1 are the bare Yukawa-couplings, $\tau_a, (a = 1, 2, 3)$ are Pauli-matrices for isospin and a summation over repeated indices a is understood. The four-nucleon interactions are obtained after integrating over the auxiliary fields according to

$$\int_{-\infty}^{\infty} d\phi\, \exp\{-\phi^2 - C\,\phi(\tilde{\psi}\psi)\} = \sqrt{\pi}\, \exp\{\frac{C^2}{4}\,(\tilde{\psi}\psi)^2\}\,. \tag{4}$$

In Ref. [15] block fields were introduced in order to separate the physical cut-off due to the extended nature of hadrons from the inherent lattice cut-off given by the inverse of the lattice spacing a. In the present paper the block fields are not introduced and there is a unique lattice cut-off. The (straightforward) introduction of the block fields is left for future work.

For the creation of sequences of interacting scalar fields $\phi_x^{(0)},\ \phi_{ax}^{(1)}$ the *two-step Polynomial Hybrid Monte Carlo* TSPHMC [26, 27, 28] algorithm is used which is a suitably adapted version of the original HMC [29] and, in particular, PHMC [30] algorithms.

2.2 Numerical simulation results

The numerical simulations are performed on a $8^3 \cdot 32$ lattice. This kind of lattices can be simulated on PC's (in our case on the PC cluster of the DESY theory group). The number of trajectories in the simulation samples is at least 5000, in some cases up to 15000. The nucleon mass m_N and the average lengths squared of the scalar fields

$$\Phi_0 \equiv \left\langle \frac{1}{N_x} \sum_x \phi_x^{(0)}\phi_x^{(0)} \right\rangle\,, \qquad \Phi_1 \equiv \left\langle \frac{1}{N_x} \sum_x \phi_{ax}^{(1)}\phi_{ax}^{(1)} \right\rangle\,. \tag{5}$$

are determined as functions of the three bare parameters κ, C_0, C_1. (N_x denotes the number of lattice sites.)

The results are summarized in Tables 1-4 and illustrated in Figures 1-6. In general, the nucleon mass is increasing for increasing C_0 and, somewhat surprisingly, decreasing for increasing C_1. The decrease for increasing hopping parameter is expected since $(2\kappa)^{-1}$ is, apart from an additive shift due to renormalization, the bare nucleon mass. This is well displayed by Fig. 3 which shows that for some *critical hopping parameter* $\kappa = \kappa(C_0, C_1)$ the nucleon mass becomes very small. (It is expected that in the infinite volume limit it becomes actually zero.) This is important if one wants to perform simulations in the small lattice spacing limit.

It is an interesting question what kind of behaviour is observed if the nucleon mass is divided by the expectation value of the average length of the isoscalar field $\langle \Phi_0 \rangle^{1/2}$. As shown by Figs. 4-5, for small C_0 this ratio is approximately constant, but for larger values of C_0 there is a moderate increase. For fixed C_0 and C_1 as a function of the hopping parameter the average field length does not change much. As a consequance, the qualitative behaviour in Figs. 3 and 6 is similar.

3 Conclusion and outlook

An important outcome of the performed unquenched simulations is the absence of any *exceptional configurations* with very small eigenvalues of the fermion matrix. No such configurations occured even at the strongest bare couplings which are much higher than the ones reached in Ref. [15]. The next goal should be to determine the renormalized four-nucleon couplings or, for instance, to tune the values of the dimensionless quantities $a_0 M_N$ and Δ/m_N where a_0 denotes the scattering length in the ${}^1S_0$ channel and Δ is the deuterium binding energy. This goes beyond the scope of this paper but is planned for future work.

From the theoretical point of view it is an interesting question whether the tuning of the renormalized couplings to their physical values is possible at all by changing the values of the bare couplings C_0 and C_1. The model studied in this paper is a special case of a renormalizable Higgs-Yukawa model where the kinetic terms of the scalar fields are omitted and the bare quartic self-couplings of the scalar fields are set to zero. These terms are all dynamically generated by the four-nucleon interactions. This means that the model investigated in this paper explores a subspace in the space of renormalized couplings of the complete renormalizable Higgs-Yukawa model. Higgs-Yukawa models in general are expected to have a trivial continuum limit with all renormalized couplings equal to zero. Therefore, in the complete Yukawa-model and also in the subspace explored in this paper there is a lattice spacing (i.e. cut-off) dependent upper limit on the renomalized couplings which tend to zero if the lattice spacing goes to zero. (Zero lattice spacing means that the nucleon mass

in lattice units am_N is zero.)

The model studied in this paper is, of course, incomplete and does not properly describe the nucleon interactions. First of all the pion field with its Yukawa interaction to the nucleons has to be introduced. Since the pion is even lighter than the nucleon, its kinetic term has to be included together with the quartic self interaction. For a complete description of the nuclear interactions further non-renormalized couplings have to be introduced which are generated within the framework of the chiral effective theory [3, 4], which served as a basis of previous investigations of nuclear physics, for instance, in [5]-[14].

A further step towards a precise description of nuclear physics with Monte Carlo methods is to control lattice artifacts introduced by the discrete lattice which break Lorentz symmetry. One possibility is to introduce higher dimensional (non-renormalizable) couplings to compensate for the lattice artifacts within the framework of *improved lattice actions* [31]-[33]. Of course, in this way a large number of couplings has to be introduced and properly tuned. Therefore, this approach becomes at some point rather cumbersome. Another possibility is to introduce block fields [15] which mimic the extended nature of hadrons (nucleons and pion) and introduce by their finite space-time extensions a natural cut-off in momentum space. In this way the physical cut-off can be separated from the lattice cut off and a small lattice spacing limit can be defined keeping the physical cut-off at its desired physical value.

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Tables

Table 1: *Numerical simulation results on* $8^3 \cdot 32$ *lattice for* $\kappa = 0.10$ *and* $C_1 = 0.05, 0.10$. *Statistical errors in last digits are given in parentheses.*

κ	C_0	C_1	$\langle \Phi_0 \rangle$	$\langle \Phi_1 \rangle$	am_N
0.10	0.01	0.05	0.501442(86)	1.48565(15)	0.68519(10)
0.10	0.05	0.05	0.53377(10)	1.48538(16)	0.70653(37)
0.10	0.10	0.05	0.62883(12)	1.48634(16)	0.76671(40)
0.10	0.15	0.05	0.77137(15)	1.48714(16)	0.85493(57)
0.10	0.20	0.05	0.94305(17)	1.48868(15)	0.96010(72)
0.10	0.25	0.05	1.12759(19)	1.48929(15)	1.06971(72)
0.10	0.30	0.05	1.31323(20)	1.49048(16)	1.1813(10)
0.10	0.35	0.05	1.49272(22)	1.49126(15)	1.2927(10)
0.10	0.40	0.05	1.66176(23)	1.49255(17)	1.39602(80)
0.10	0.50	0.05	1.96256(27)	1.49353(17)	1.5840(14)
0.10	0.01	0.10	0.501517(84)	1.44292(14)	0.65804(19)
0.10	0.05	0.10	0.534201(93)	1.44379(14)	0.67974(28)
0.10	0.10	0.10	0.630929(42)	1.446002(51)	0.74205(18)
0.10	0.15	0.10	0.77541(16)	1.44939(16)	0.83309(79)
0.10	0.20	0.10	0.949356(51)	1.453549(45)	0.94291(20)
0.10	0.25	0.10	1.13598(18)	1.45796(14)	1.05644(79)
0.10	0.30	0.10	1.32251(21)	1.46198(16)	1.17402(64)
0.10	0.35	0.10	1.50271(21)	1.46593(14)	1.28402(95)
0.10	0.40	0.10	1.67156(24)	1.46914(17)	1.3872(10)

Table 2: *Numerical simulation results on* $8^3 \cdot 32$ *lattice for* $\kappa = 0.10$ *and* $C_1 = 0.20, 0.30$. *Statistical errors in last digits are given in parentheses.*

κ	C_0	C_1	$\langle \Phi_0 \rangle$	$\langle \Phi_1 \rangle$	am_N
0.10	0.01	0.20	0.501340(96)	1.28479(13)	0.5629(12)
0.10	0.05	0.20	0.536649(99)	1.28722(16)	0.58162(80)
0.10	0.10	0.20	0.639301(76)	1.296000(78)	0.65369(54)
0.10	0.15	0.20	0.79218(16)	1.30891(13)	0.75732(85)
0.10	0.20	0.20	0.97365(12)	1.32375(10)	0.87765(60)
0.10	0.25	0.20	1.16692(22)	1.33980(14)	1.00478(60)
0.10	0.30	0.20	1.35767(24)	1.35509(15)	1.12985(85)
0.10	0.35	0.20	1.53994(24)	1.36975(15)	1.24829(94)
0.10	0.40	0.20	1.70999(27)	1.38275(17)	1.35859(87)
0.10	0.01	0.30	0.501390(95)	1.06681(11)	0.4296(47)
0.10	0.05	0.30	0.53978(12)	1.07226(11)	0.4501(25)
0.10	0.10	0.30	0.65177(14)	1.08780(11)	0.5431(36)
0.10	0.15	0.30	0.81674(18)	1.11161(12)	0.6495(19)
0.10	0.20	0.30	1.01076(22)	1.14042(14)	0.78928(71)
0.10	0.25	0.30	1.21305(26)	1.17062(14)	0.92980(98)
0.10	0.30	0.30	1.41081(29)	1.20080(16)	1.0690(10)
0.10	0.35	0.30	1.59643(29)	1.22882(16)	1.1968(13)
0.10	0.40	0.30	1.76870(31)	1.25445(18)	1.3087(37)

Table 3: *Numerical simulation results on* $8^3 \cdot 32$ *lattice for* $\kappa = 0.11$ *and* $C_1 = 0.10$. *Statistical errors in last digits are given in parentheses.*

κ	C_0	C_1	$\langle\Phi_0\rangle$	$\langle\Phi_1\rangle$	am_N
0.11	0.01	0.10	0.501270(83)	1.44445(14)	0.4281(50)
0.11	0.05	0.10	0.533467(94)	1.44488(14)	0.4436(36)
0.11	0.10	0.10	0.62864(13)	1.44667(15)	0.5009(15)
0.11	0.15	0.10	0.77138(15)	1.44977(15)	0.6005(12)
0.11	0.20	0.10	0.94432(16)	1.45419(15)	0.72170(73)
0.11	0.25	0.10	1.13103(15)	1.45808(13)	0.85157(58)
0.11	0.30	0.10	1.31808(22)	1.46208(16)	0.97838(74)
0.11	0.35	0.10	1.49865(21)	1.46600(15)	1.10036(79)
0.11	0.40	0.10	1.66819(24)	1.46932(16)	1.21527(81)

Table 4: *Numerical simulation results on* $8^3 \cdot 32$ *lattice for* $C_1 = 0.05$ *and* $C_0 = 0.40, 0.60$. *Statistical errors in last digits are given in parentheses.*

κ	C_0	C_1	$\langle \Phi_0 \rangle$	$\langle \Phi_1 \rangle$	am_N
0.10	0.40	0.05	1.66176(23)	1.49255(17)	1.39402(80)
0.11	0.40	0.05	1.65810(23)	1.49209(17)	1.2230(13)
0.12	0.40	0.05	1.65354(24)	1.49221(17)	1.04973(95)
0.13	0.40	0.05	1.64713(23)	1.49224(17)	0.87697(84)
0.14	0.40	0.05	1.63763(23)	1.49233(17)	0.7033(13)
0.15	0.40	0.05	1.62421(25)	1.49253(17)	0.5154(20)
0.16	0.40	0.05	1.60449(25)	1.49267(18)	0.3612(94)
0.10	0.60	0.05	2.2115(24)	1.49573(13)	1.7512(36)
0.11	0.60	0.05	2.21459(29)	1.49453(14)	1.5983(31)
0.12	0.60	0.05	2.21269(31)	1.49462(18)	1.4567(11)
0.13	0.60	0.05	2.20967(33)	1.49470(17)	1.3159(11)
0.14	0.60	0.05	2.20585(32)	1.49470(18)	1.1725(19)
0.15	0.60	0.05	2.20051(32)	1.49471(18)	1.0368(14)
0.16	0.60	0.05	2.19391(27)	1.49474(19)	0.89612(85)
0.17	0.60	0.05	2.18459(29)	1.49474(19)	0.7542(11)
0.18	0.60	0.05	2.17155(28)	1.49500(19)	0.6109(21)
0.19	0.60	0.05	2.15482(30)	1.49495(19)	0.4664(40)

Figures

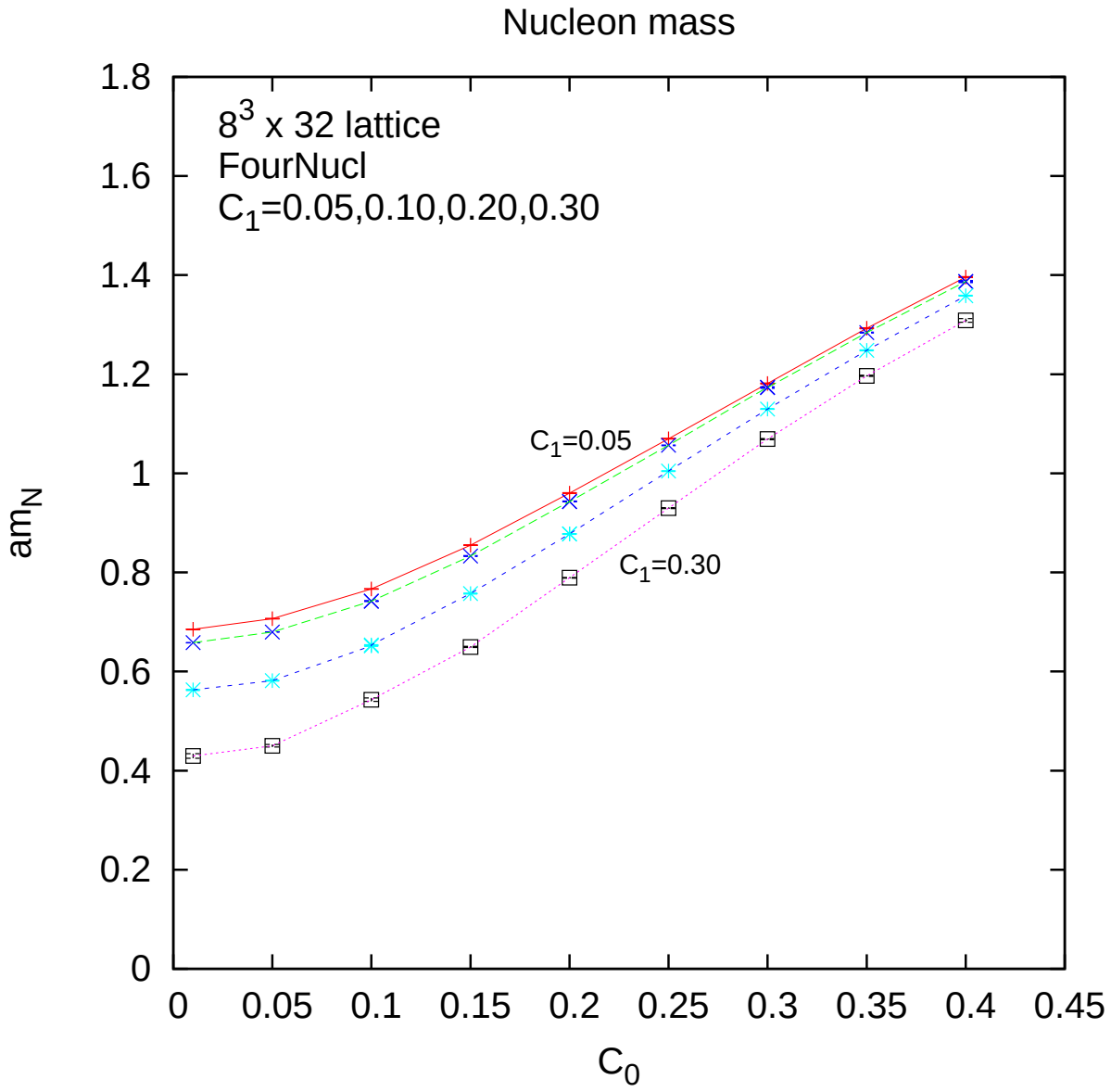

Figure 1: *The nucleon mass as function of the coupling C_0 for $\kappa = 0.10$ and different values of C_1. The lines are drawn to guide the eyes.*

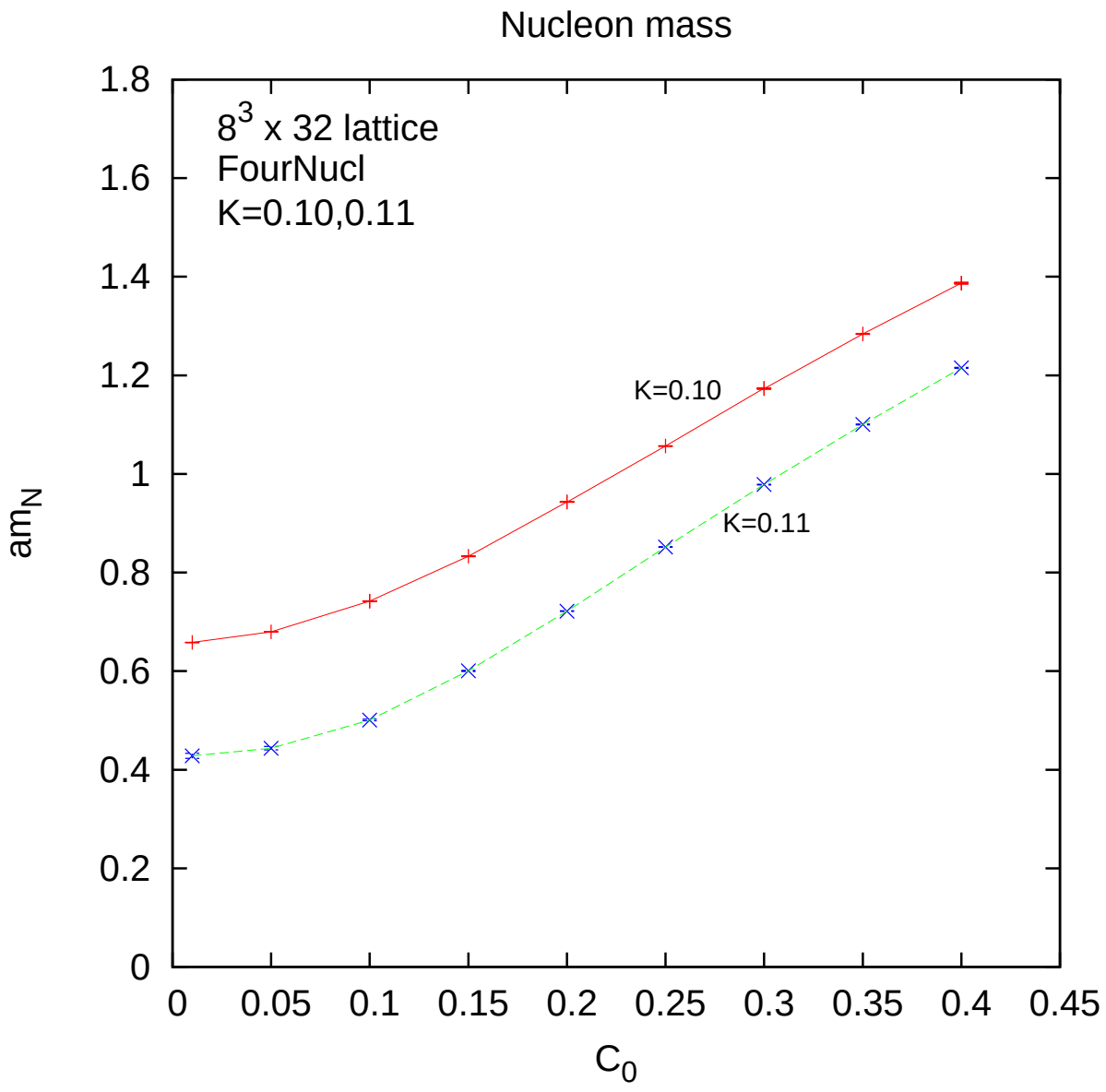

Figure 2: *The nucleon mass as function of the coupling C_0 for $\kappa = 0.10$ and $\kappa = 0.11$. The lines are drawn to guide the eyes.*

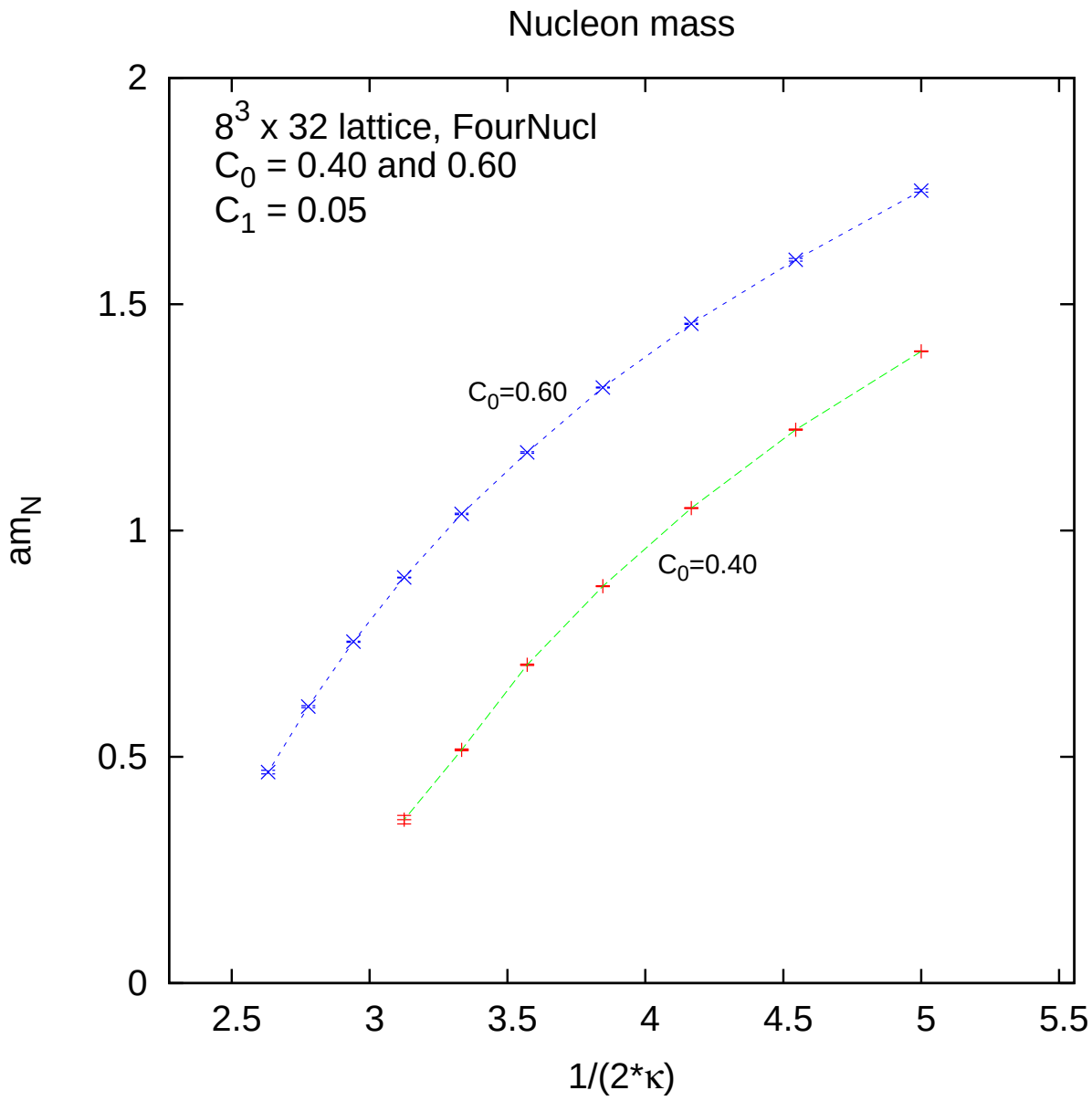

Figure 3: *The nucleon mass as function of the bare mass parameter* $(2\kappa)^{-1}$ *for* $C_1 = 0.05$ *and for* $C_0 = 0.40$ *and* $C_0 = 0.60$. *The lines are drawn to guide the eyes.*

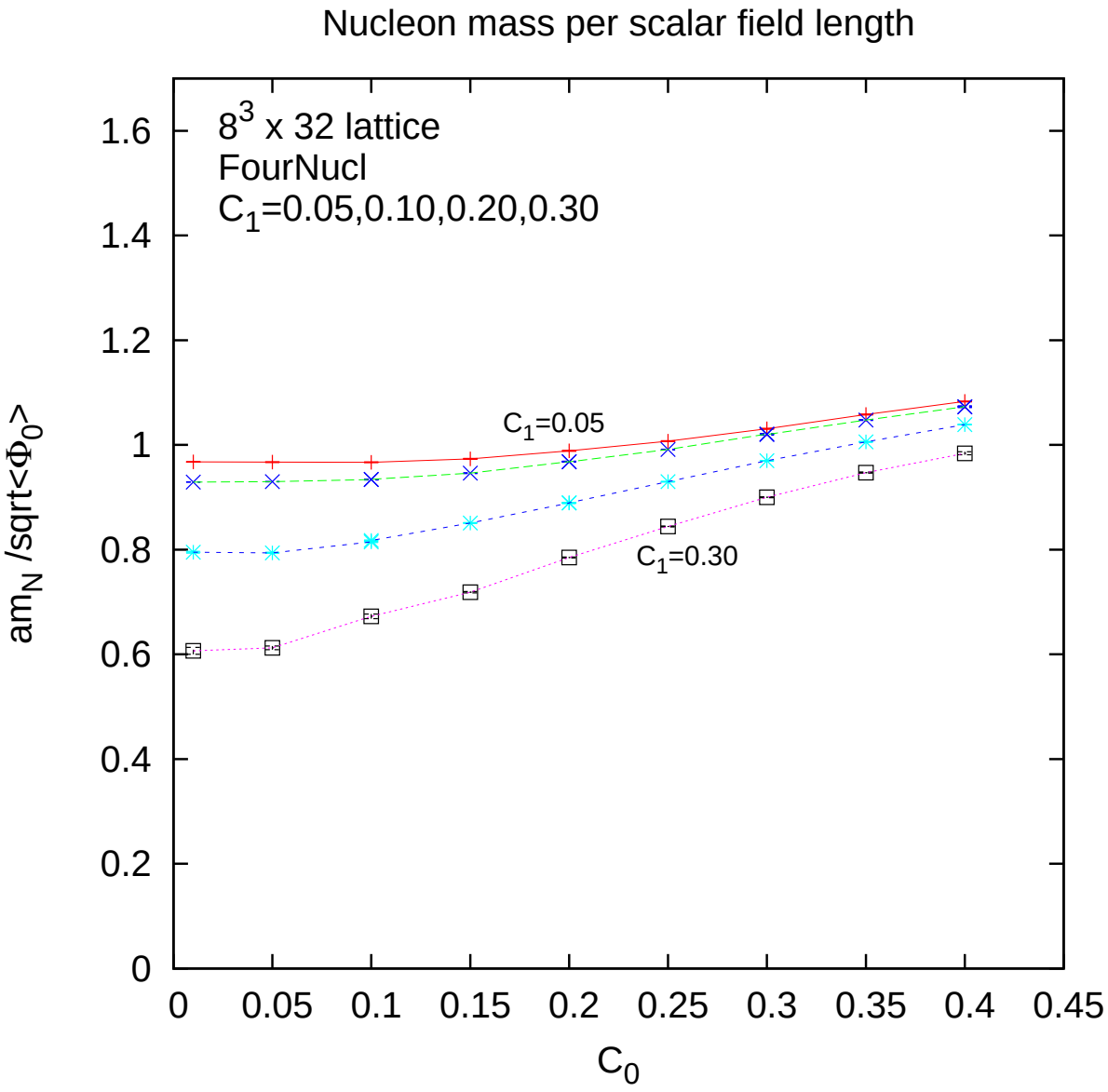

Figure 4: *The nucleon mass divided by the expectation value of the average length of the isoscalar field* $\langle \Phi_0 \rangle^{1/2}$ *as function of the coupling* C_0 *for* $\kappa = 0.10$ *and different values of* C_1*. The lines are drawn to guide the eyes.*

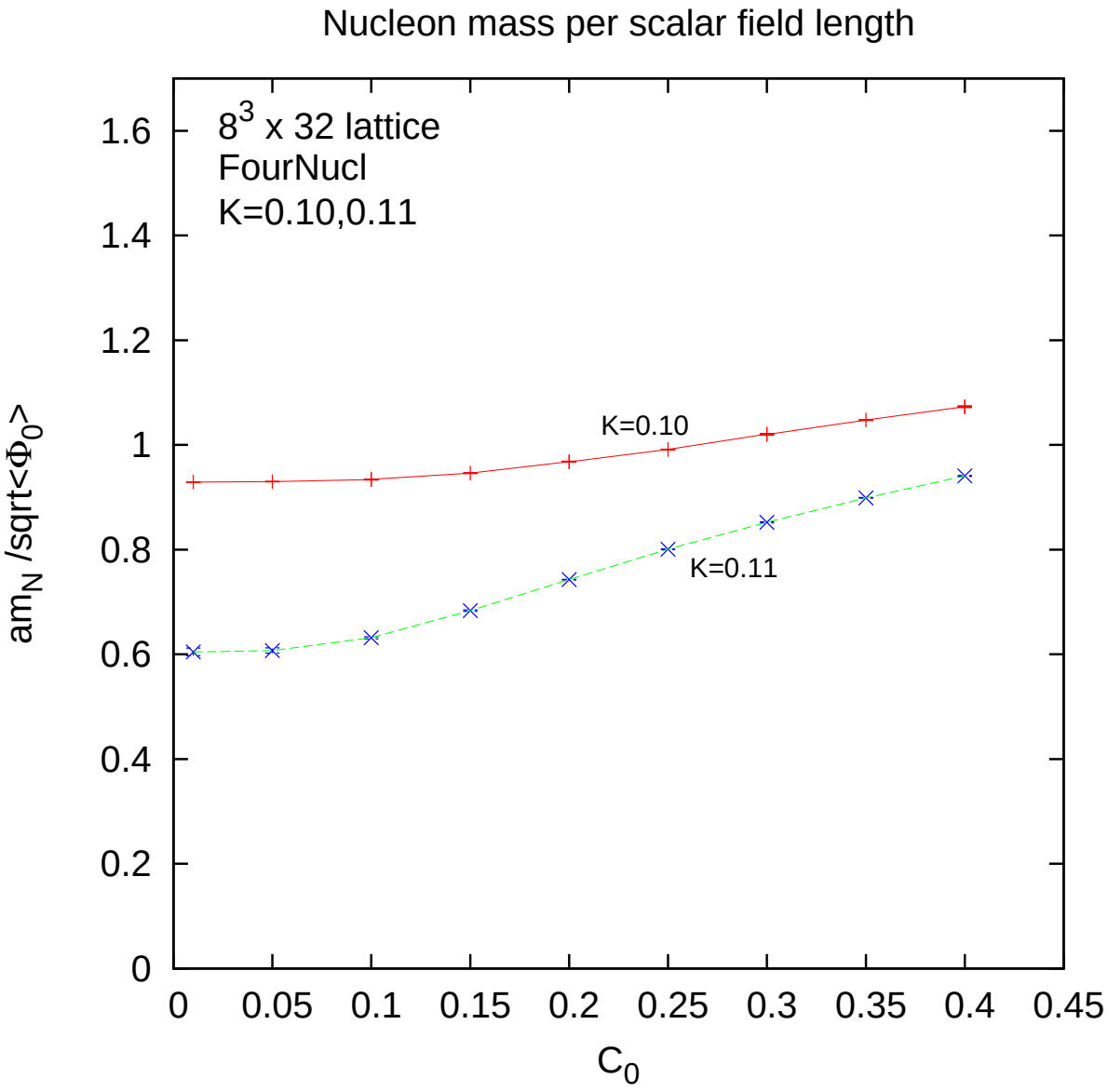

Figure 5: *The nucleon mass divided by the expectation value of the average length of the isoscalar field* $\langle \Phi_0 \rangle^{1/2}$ *as function of the coupling* C_0 *for* $\kappa = 0.10$ *and* $\kappa = 0.11$. *The lines are drawn to guide the eyes.*

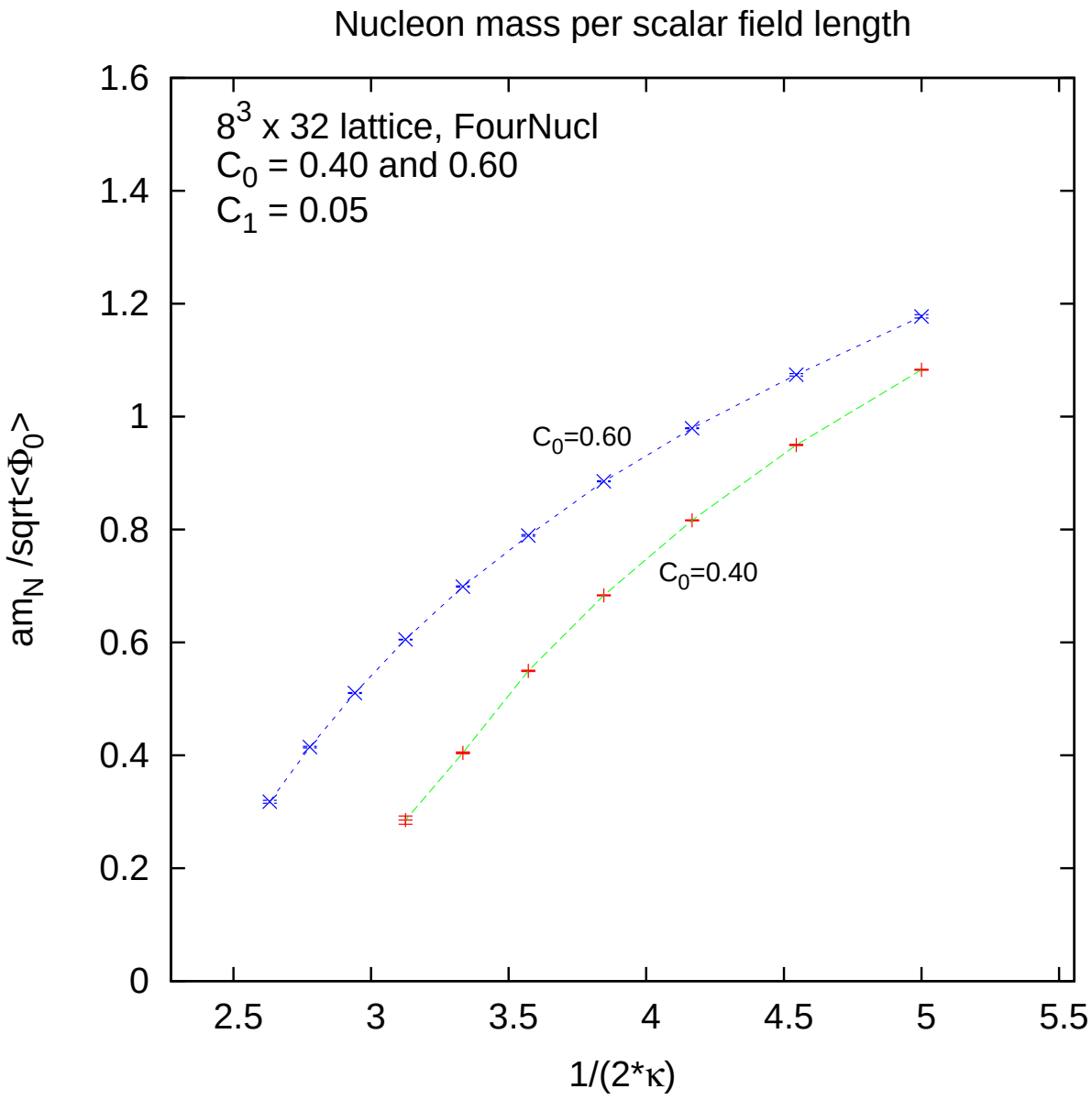

Figure 6: *The nucleon mass divided by the expectation value of the average length of the isoscalar field* $\langle\Phi_0\rangle^{1/2}$ *as function of the bare mass parameter* $(2\kappa)^{-1}$ *for* $C_1 = 0.05$ *and for* $C_0 = 0.40$ *and* $C_0 = 0.60$. *The lines are drawn to guide the eyes.*